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Sorting Category: 13.2 (Computation/Simulation)

Quantum Dot Modeling using NEMO 3-D GERHARD KLIMECK, Jet Propulsion Laboratory, California Institute of Technology, R. C. BOWEN, JPL, T. B. BOYKIN, University of Alabama in Huntsville, Huntsville, AL 35899 — Nano-scaled electronic devices are characterized by material and charge density variations on the length scale of a few atoms. Typical strucure sizes range from few hundreds to tens of millions of atoms. A nanoelectronic modeling tool (NEMO-3D) that enables the analysis of the electronic structure of arbitrarily shaped quantum dots of arbitrary composistion and crystal structure is being developed. A tight-binding model using s, p, and d orbitals is used to represent the electronic strucutre of realistically sized quantum dots. Parallel algorithms are employed to compute the single electron states in systems as big as 10 million atoms. An overview of the simulator and first results dealing with strain, alloyed dots and interface interdiffusion will be presented. More information about the work can be found at this website http://hpc.jpl.nasa.gov/PEP/gekco.

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